Textures and Microstructures, Vol. 32, pp. 309–319
Reprints available directly from the publisher
Photocopying permitted by license only

CALCULATION OF MICROSTRESSES IN TEXTURED POLYCRYSTALS WITH CUBIC CRYSTAL SYMMETRY

E.A. MITYUSHOV* and S.A. BERESTOVA

Ural State Technical University, 19 Mira, Ekaterinburg 620002, Russia

(Received in final form 28 September 1997)

The problem of the analytic determination of microstresses in textured polycrystals with cubic symmetry under general static loading has been solved. The solution is based on the expansion of macroscopic and microscopic stress fields into hydrostatic and deviatoric portions. This essentially simplifies the description of microstresses in polycrystals.

Keywords: Stresses in grain; Inhomogeneity; Texture

1. INTRODUCTION

Under rejection of the hypothesis of a homogeneous medium, macrostresses in the textured polycrystal are determined as the average of microstresses in grains of a polycrystal over a representative volume of the medium containing a sufficiently large amount of the grains. Microstresses are determined by the applied macrostresses and the distinction between the effective and local values of the elastic constants. The well-known models of Sachs and Reuss (Taylor and Voigt) are based on the assumption of homogeneity of stresses (strains) in the sample. Consequently these models do not consider the influence of surrounding grains and texture on the stresses in the grains. The estimation of the influence of texture and interactions between grains on the microstresses under various orientations of external load is the topic of this paper.

* Corresponding author.

Polycrystals with cubic crystal symmetry are considered. For clear description of the interaction between grains and the influence of texture on the microscopic stresses, microstresses are found in the grains of non-textured material and a polycrystal with special texture. The obtained results are compared with the data for a homogeneous material (i.e. a single crystal). The solution is based on the known effective values of elastic characteristics of the polycrystal. For a quasi-isotropic system, this is the Aleksandrov's solution (Aleksandrov, 1965). For a textured material, these are exact elastic constants of the two-component texture (001)[100] + (001)[110] (Mityushov and Berestova, 1995).

2. DETERMINATION OF MICROSTRESSES IN GRAINS OF TEXTURED POLYCRYSTALS

Local stresses in a non-textured (quasi-isotropic) material are found using Eshelby's solution (Eshelby, 1957) for the deformation of an elastic spherical grain of cubic symmetry embedded in an infinite homogeneous matrix.

Let ε^c be the constrained strain of a bigger size grain from material of the matrix with elastic characteristics c^*. Equate the stress in this grain under the given uniform strain of the polycrystal $\langle\varepsilon\rangle$ to the stress in the cubic symmetry grain with properties c under the same uniform strain (Shermergor, 1977)

$$c(\varepsilon^c + \langle\varepsilon\rangle) = c^*\left(\varepsilon^c + \langle\varepsilon\rangle - \varepsilon^T\right). \tag{2.1}$$

Here ε^T is the tensor of incompatibility of strains.

Based on Eshelby's solution, the tensor of the constrained strain and the tensor of incompatibility of strains are related to each other in the following manner:

$$\varepsilon^c = N\varepsilon^T \quad \text{or} \quad \varepsilon^T = W\varepsilon^c. \tag{2.2}$$

The components of the Eshelby's tensor $N = W^{-1}$ are given by

$$N_{ijkl} = \frac{1}{2} c^*_{pqkl} \int_{v_0} \left[\frac{\partial^2 G_{pi}(x, x')}{\partial x_{(j)} \partial x_q} + \frac{\partial^2 G_{pj}(x, x')}{\partial x_{(i)} \partial x_q}\right] \mathrm{d}v, \tag{2.3}$$

where $G_{pi}(x, x')$ is the Green's tensor of the infinite homogeneous medium; v_0 is the volume occupied by the grain.

Taking into consideration that strains in the grain are equal to the sum of the constrained and uniform strains ($\varepsilon = \varepsilon^c + \langle\varepsilon\rangle$), from Eq. (2.1) in terms of the relation (2.2) we have

$$c\varepsilon = c^*[\varepsilon - W(\varepsilon - \langle\varepsilon\rangle)]. \tag{2.4}$$

From Eq. (2.4) we obtain

$$\left[(c^*)^{-1}c - I\right]\varepsilon = W(\langle\varepsilon\rangle - \varepsilon), \tag{2.5}$$

where I is the fourth rank unit tensor detined by

$$I_{ijkl} = \tfrac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{2.6}$$

Hence

$$\langle\varepsilon\rangle - \varepsilon = N\left[(c^*)^{-1}c - I\right]\varepsilon. \tag{2.7}$$

As a result, the strain tensor of the grain is

$$\varepsilon = \left\{I + N\left[(c^*)^{-1}c - I\right]\right\}^{-1}\langle\varepsilon\rangle. \tag{2.8}$$

Since averages of strain and stress tensors taken over the volume of a polycrystal are related through the generalised Hooke's law

$$\langle\varepsilon\rangle = s^*\langle\sigma\rangle, \tag{2.9}$$

then

$$s\sigma = \{I + N[s^*c - I]\}^{-1}s^*\langle\sigma\rangle \quad \text{or} \quad \sigma = c\{I + N[s^*c - I]\}^{-1}s^*\langle\sigma\rangle. \tag{2.10}$$

Expression (2.10) is a tensor equation for determination of microstresses. However, direct application of the expression is difficult due to its tensoral nature.

Equation (2.10) can be rewritten using the expansion of the unit tensor given by Morawiec (Morawiec, 1994)

$$I = E_1 + E_2 + E_3, \tag{2.11}$$

where

$$(E_1)_{ijkl} = \tfrac{1}{3}\delta_{ij}\delta_{kl}, \qquad (E_2)_{ijkl} = \sum_{m=1}^{3} \delta_{i(m)}\delta_{j(m)}\delta_{k(m)}\delta_{l(m)} - \tfrac{1}{3}\delta_{ij}\delta_{kl},$$
$$(E_3)_{ijkl} = I_{ijkl} - \sum_{m=1}^{3} \delta_{i(m)}\delta_{j(m)}\delta_{k(m)}\delta_{l(m)}. \tag{2.12}$$

The above tensors E_i satisfy the orthogonality relation $E^iE^j = \delta_{ij}E^{(i)}$.

The stress tensor in Eq. (2.10) can now be represented in the following expansion of independent components:

$$\sigma = I\sigma = E_1\sigma + E_2\sigma + E_3\sigma = \sigma_1 + \sigma_2 + \sigma_3, \tag{2.13}$$

where

$$\sigma_1 = \begin{pmatrix} \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33}) & 0 & 0 \\ 0 & \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33}) & 0 \\ 0 & 0 & \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33}) \end{pmatrix}$$

is the hydrostatic portion of the stress tensor,

$$\sigma_2 = \begin{pmatrix} \frac{1}{3}(\sigma_{11} - \sigma_{22}) + \frac{1}{3}(\sigma_{11} - \sigma_{33}) & 0 & 0 \\ 0 & \frac{1}{3}(\sigma_{22} - \sigma_{33}) + \frac{1}{3}(\sigma_{22} - \sigma_{11}) & 0 \\ 0 & 0 & \frac{1}{3}(\sigma_{33} - \sigma_{11}) + \frac{1}{3}(\sigma_{33} - \sigma_{22}) \end{pmatrix},$$

$$\sigma_3 = \begin{pmatrix} 0 & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & 0 & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_0 \end{pmatrix},$$

$\sigma_2 + \sigma_3$ is the deviatoric portion of the stress tensor.

Tensors of elastic characteristics are represented with the help of this expansion of the unit tensor in the form

$$c = Ic = E_1c + E_2c + E_3c = 3KE_1 + (c_{11} - c_{12})E_2 + 2c_{44}E_3, \quad (2.14)$$

where c_{ij} are single crystal data in matrix notation,

$$s^* = Is^* = E_1s^* + E_2s^* + E_3s^* = \frac{1}{3K}E_1 + \frac{1}{2\mu^*}E_2 + \frac{1}{2\mu^*}E_3, \quad (2.15)$$

where $\mu^* = c_{44}^{3/5}((c_{11} - c_{12})/2)^{2/5}$ is Aleksandrov's solution (Aleksandrov, 1965) obtained for a non-textured polycrystal with cubic crystal symmetry, and $K = \frac{1}{3}(c_{11} + 2c_{12})$ is the bulk modulus.

The Eshelby's tensor is expanded into members in a similar manner

$$N = IN = E_1N + E_2N + E_3N = 3N_1E_1 + 2N_2E_2 + 2N_3E_3. \quad (2.16)$$

In this case independent coefficients of expanded tensors are determined by bulk modulus and Poisson's coefficient ν^* of the matrix material,

$$\begin{aligned} N_1 &= \frac{1 + \nu^*}{9(1 - \nu^*)} = \frac{K}{3K + 4\mu^*}, \\ N_2 = N_3 &= \frac{4 - 5\nu^*}{15(1 - \nu^*)} = \frac{3(K + 2\mu^*)}{5(3K + 4\mu^*)}. \end{aligned} \quad (2.17)$$

Using the representation, Eq. (2.10) is simplified because the tensor relationship in terms of the orthogonality expansion of the unit tensor is reduced to scalar equations for determination of the unknown coefficients.

As a result, Eq. (2.10) can be written in the form

$$\sigma = (\alpha_1E_1 + \alpha_2E_2 + \alpha_3E_3)\langle\sigma\rangle = \alpha_1\langle\sigma_1\rangle + \alpha_2\langle\sigma_2\rangle + \alpha_3\langle\sigma_3\rangle, \quad (2.18)$$

where the coefficients are

$$\begin{aligned} \alpha_1 &= 1, \qquad \alpha_2 = \frac{1}{(2\mu^*/(c_{11} - c_{12}))(1 - 2N_2) + 2N_2}, \\ \alpha_3 &= \frac{1}{(\mu^*/c_{44})(1 - 2N_3) + 2N_3}. \end{aligned} \quad (2.19)$$

3. DETERMINATION OF MICROSTRESSES IN GRAINS OF TEXTURED POLYCRYSTAL

Determination of microstresses in a textured polycrystal with cubic crystal symmetry has been realised for the example of a two-component texture (001)[100] + (001)[110], where the components are taken in equal concentrations. The polycrystal system is a macro-transverse–isotropic system, i.e. the system has a plane of symmetry.

For the two-component medium, the compliance tensor at an arbitrary point of the system can be written as

$$s = \lambda(s_1 - s_2) + s_2, \tag{3.1}$$

where s_1 and s_2 are the compliance tensors for the orientations [100] and [110], respectively, and λ is a random indicator function that indicates which texture component is present. $\langle\lambda\rangle$ is equal to the volume content of the first component, and in the equal volume case $\langle\lambda\rangle = 1/2$.

Further, for determining the average stress over a volume which is occupied by the separate orientation, we use the Hooke's law for an arbitrary point of the system. The condition (3.1) allows us to write the Hooke's law in the form

$$\varepsilon = s_2\sigma + \lambda(s_1 - s_2)\sigma. \tag{3.2}$$

Averaging over the whole volume of the textured sample and using the properties of the indicator flinction one has

$$\langle\varepsilon\rangle = s_2\langle\sigma\rangle + \tfrac{1}{2}(s_1 - s_2)\langle\sigma\rangle_1, \tag{3.3}$$

where $\langle\sigma\rangle$ is the average stress tensor over the volume which is occupied by the first component. Since polycrystal volume averages of the stress and strain are related with the effective compliance tensor through the generalised Hooke's law (2.9), the equation for determining the average stress tensor over the volume which is occupied by the first component is given by

$$(s^* - s_2)\langle\sigma\rangle = \tfrac{1}{2}(s_1 - s_2)\langle\sigma\rangle_1. \tag{3.4}$$

The effective elastic characteristics of the system are found from the exact solution (Mityushov and Berestova, 1995). The solution was obtained from the invariance condition of the system transformation for rotations of $\pi/4$ about the general symmetry axis of the material,

$$\begin{gathered} s_{11}^{*}=\tfrac{1}{2}(s_{11}+s_{12})+\tfrac{1}{4}\sqrt{2(s_{11}-s_{12})s_{44}}, \\ s_{12}^{*}=\tfrac{1}{2}(s_{11}+s_{12})-\tfrac{1}{4}\sqrt{2(s_{11}-s_{12})s_{44}}, \\ s_{33}^{*}=s_{11}, \quad s_{13}^{*}=s_{12}^{*}, \quad s_{44}^{*}=s_{44}, \quad s_{66}^{*}=\sqrt{2(s_{11}-s_{12})s_{44}}, \end{gathered} \tag{3.5}$$

where s_{ij} are single crystal data in matrix notation.

Since the system has specific structure from the relations (3.4) and (3.5) we have found shear stresses in the (100) and (110) crystallographic planes of the (001)[100] orientation,

$$\begin{aligned} \langle\sigma_{12}\rangle_1 &= -\frac{s_{66}^{*}-s_{44}-2s}{s}\langle\sigma_{12}\rangle = -\frac{\sqrt{2(s_{11}-s_{12})s_{44}}-s_{44}-2s}{s}\langle\sigma_{12}\rangle, \\ \frac{\langle\sigma_{11}\rangle_1-\langle\sigma_{22}\rangle_1}{2} &= \frac{(s_{11}^{*}-s_{11}-s_{12}^{*}+s_{12}+s)}{s}(\langle\sigma_{11}\rangle-\langle\sigma_{22}\rangle) \\ &= \frac{\sqrt{2(s_{11}-s_{12})s_{44}}-2(s_{11}-s_{12})+2s)}{2s}(\langle\sigma_{11}\rangle-\langle\sigma_{22}\rangle), \end{aligned} \tag{3.6}$$

where $s=s_{11}-s_{12}-\frac{1}{2}s_{44}$.

Similarly the expression for the average stress tensor $\langle\sigma\rangle_2$ over the volume which is occupied by the second component (001)[110] can be found by simple substitution of index $1\leftrightarrow 2$. Obviously, the following equation must be satisfied:

$$\langle\sigma\rangle=\tfrac{1}{2}(\langle\sigma\rangle_1+\langle\sigma\rangle_2). \tag{3.7}$$

The tensor $\langle\sigma\rangle_1$ for the transverse–isotropic material can be represented in the expanded form

$$\langle\sigma\rangle_1=\alpha_1\langle\sigma_1\rangle+\alpha_2\langle\sigma_2\rangle+\alpha_3\langle\sigma_3\rangle+\alpha_4\langle\sigma_4\rangle+\alpha_5\langle\sigma_5\rangle+\alpha_6\langle\sigma_6\rangle+\alpha_7\langle\sigma_7\rangle, \tag{3.8}$$

where $\langle\sigma_1\rangle$ is the hydrostatic portion of the tensor,

$$\langle\sigma_2\rangle = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{3}(\langle\sigma_{22}\rangle - \langle\sigma_{33}\rangle) & 0 \\ 0 & 0 & \frac{1}{3}(\langle\sigma_{33}\rangle - \langle\sigma_{22}\rangle) \end{pmatrix},$$

$$\langle\sigma_3\rangle = \begin{pmatrix} \frac{1}{3}(\langle\sigma_{11}\rangle - \langle\sigma_{33}\rangle) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3}(\langle\sigma_{33}\rangle - \langle\sigma_{11}\rangle) \end{pmatrix},$$

$$\langle\sigma_4\rangle = \begin{pmatrix} \frac{1}{3}(\langle\sigma_{11}\rangle - \langle\sigma_{22}\rangle) & 0 & 0 \\ 0 & \frac{1}{3}(\langle\sigma_{22}\rangle - \langle\sigma_{11}\rangle) & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\langle\sigma_5\rangle = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \langle\sigma_{23}\rangle \\ 0 & \langle\sigma_{23}\rangle & 0 \end{pmatrix},$$

$$\langle\sigma_6\rangle = \begin{pmatrix} 0 & 0 & \langle\sigma_{13}\rangle \\ 0 & 0 & 0 \\ \langle\sigma_{13}\rangle & 0 & 0 \end{pmatrix},$$

$$\langle\sigma_7\rangle = \begin{pmatrix} 0 & \langle\sigma_{12}\rangle & 0 \\ \langle\sigma_{12}\rangle & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

In the considered case, the following coefficients of the expansion are obtained:

$$\begin{aligned} &\alpha_1 = 1, \qquad \alpha_4 = \frac{\sqrt{2(s_{11} - s_{12})s_{44}} - 2(s_{11} - s_{12}) + 2s}{s}, \\ &\alpha_5 = \alpha_6 = 1, \qquad \alpha_7 = -\frac{\sqrt{2(s_{11} - s_{12})s_{44}} - s_{44} - 2s}{s}. \end{aligned} \tag{3.9}$$

Use of these coefficients allows the estimation of the tangential stresses in the (100) and (110) crystallographic planes for each of the texture components in response to the external stress field.

This considers, in particular, the influence of the inhomogeneity of the medium on the change of the tangential stresses $\tau_{(001)[100]}$ and $\tau_{(110)[1\bar{1}0]}$ versus the application of external tensile load in the (001) plane of the fixed crystallite. The relations (3.6) in the case can be written in the form

$$\begin{aligned} \tau_{(001)[100]} &= \langle\sigma_{12}\rangle_1 = \frac{\alpha_7}{2}\sin(2\phi)\langle\sigma\rangle, \\ \tau_{(110)[1\bar{1}0]} &= \frac{\langle\sigma_{11}\rangle_1 - \langle\sigma_{22}\rangle_1}{2} = -\frac{\alpha_4}{2}\cos(2\phi)\langle\sigma\rangle, \end{aligned} \tag{3.10}$$

where $\langle\sigma\rangle$ is the external tensile load, ϕ is the angle between the tensile axis and the [001] direction.

4. SUMMARY

The ratios of the shear stresses in the planes (100), (110) and the tensile load versus the angle between the tensile axis and the direction [001] are shown in Fig. 1 for gold, lead and aluminium for the monocrystal, the quasi-isotropic polycrystal and the textured two-component polycrystal.

From these figures, it can be concluded that inhomogeneity can have a significant impact on the distribution of microstresses in grains of a polycrystal. The texture of the material and the anisotropy of the single crystal elastic properties had the most impact on the values of the local stresses. The largest inhomogeneity of stresses, which is characterised by the differences of the critical shear microstress in the inhomogeneous and homogeneous material (single crystal) are shown by materials with a high indicator of elastic anisotropy (Pb, Au). The largest differences for the (001)[110] system were achieved when the tensile axis and the [100] direction coincided, while for the (001)[100] system they were achieved when the tensile axis and the [110] direction coincided.

The obtained solution allows the estimation of the inhomogeneity of the shear stresses, as distinct from the well-known models of Sachs and Reuss. Stresses in the considered crystallographic systems of the inhomogeneous textured material are twice that of the corresponding homogeneous material. Consequently, use of the indicated models in this case yields a very rough approximation.

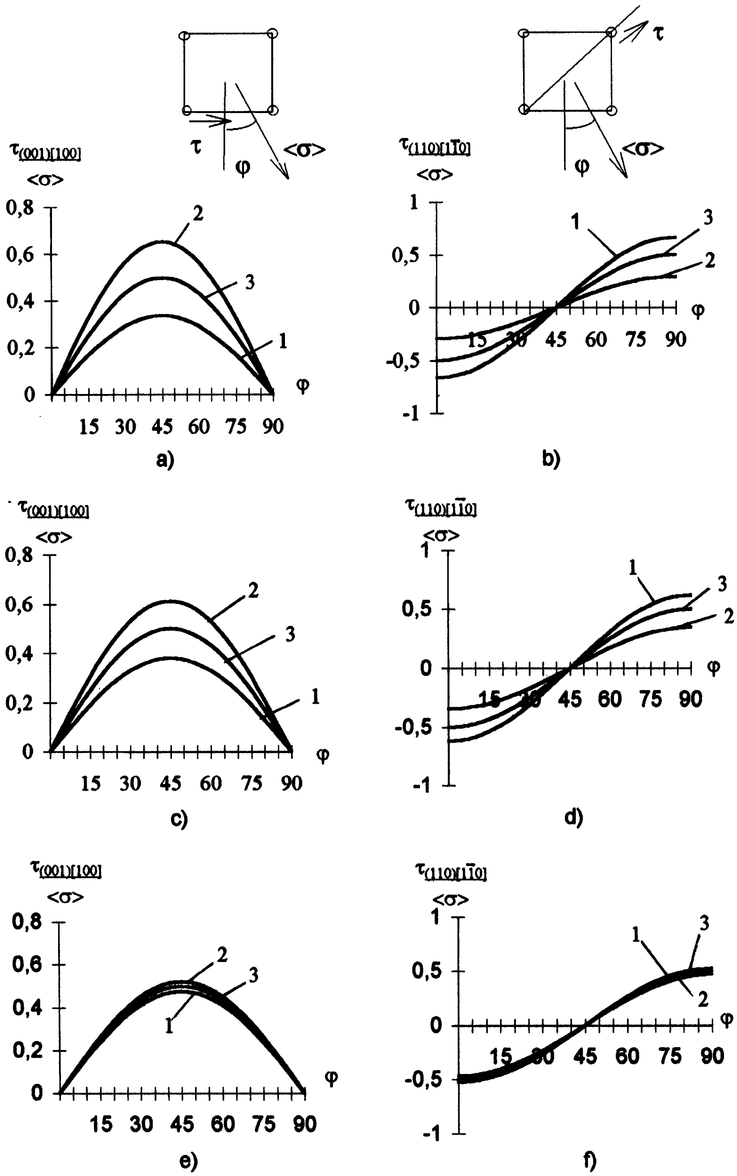

FIGURE 1 Dependence of the ratio of the tangential stresses τ for the two crystallographic systems to the tensile stress $\langle\sigma\rangle$ on the direction of its application for lead (a,b), gold (c,d) and aluminium (e,f) in textured, quasi-isotropic and homogeneous material. 1 denotes the curve obtained for textured polycrystal (001)[100]+(001)[110]; 2 is for quasi-isotropic material; 3 is for homogeneous material.

When microstresses are calculated in the textured polycrystal it is necessary to take into account the influence on the stresses in the grains not only of the external load but also of the interaction between neighbouring grains during the deformation process as well.

References

Aleksandrov, K.S. (1965) *Dokl. A. N. SSSR*, **164**, 800–803.
Eshelby, J.P. (1957) *Proc. of the Royal Society, London*, **A241**, 376–392.
Mityushov, E.A. and Berestova, S.A. (1995) *Proc. ICOTOM-11*, 830–835.
Morawiec, A. (1994) *Texture and Microstructures*, **22**, 139–167.
Shermergor, T.D. (1977) *The Theory of Elasticity of Microinhomogeneous Media.* Moscow, Nauka.